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Br.
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chain nodes :
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
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1-2 1-8 2-3 3-4 4-5 5-6 6-7 7-8
exact/norm bonds :
1-2 1-8 2-3 3-4 4-5 5-6 6-7 7-8
exact bonds :
4-9
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L3
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L5 ANSWER 50 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

```
Title
          Cyclooctatetraene derivatives from bromocyclooctatetraene
Author/Inventor
          Harmon, Claude A.; Streitwieser, Andrew, Jr.
Patent Assignee/Corporate Source
          Dep. Chem., Univ. California, Berkeley, CA, USA
Source
          Journal of Organic Chemistry (1973), 38(3), 549-51 CODEN: JOCEAH: ISSN: 0022-3263
Document Type
          Journal
Language
          English
Abstract
          N,N-Dimethylaminocyclooctatetraene, cyclopropylcyclooctatetraene, and cyclooctatetraenenitrile were prepared for the first time.
          N.N-Diethylaminocyclooctatetraene was also prepared, but rearranged to a-N,N-diethylaminostyrene, p-Anisylcyclooctatetraene,
          cyclooctatetraenealdehyde, and vinylcyclooctatetraene were prepared in greatly improved yields over previously described
          procedures.
L5 ANSWER 51 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
          Reaction of 1,3,5-cyclooctatrien-7-yne at various temperatures
Author/Inventor
          Ogliaruso, Michael A.; Lankey, Ann S.
Patent Assignee/Corporate Source
          Dep. Chem., Virginia Polytech. Nst., Blacksburg, VA, USA
Source
          Journal of Organic Chemistry (1971), 36(22), 3339-42 CODEN: JOCEAH; ISSN: 0022-3263
Document Type
          Journal
Language
          English
Abstract
          1,3,5-Cyclooctatrien-7-yne (dehydrocyclooctatetraene) was reported best prepared in ether at room temperature, to afford the
          highest yield of adduct with a trapping agent. Yields of product from the reaction of this species with a trapping agent vary
          depending upon (a) when the trapping agent is added, and, (b) the temperature employed. Contrary to previous indicated reports.
          dehydrocyclooctatetraene is best prepared and allowed to react at temps, other than room temperature
L5 ANSWER 52 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
Title
          Chloro-, bromo, and iodocyclooctatetraene. Preparation and some reactions
Author/Inventor
          Gasteiger, Johann; Gream, George E.; Huisgen, Rolf; Konz, Will E.; Schnegg, Ulrich
Patent Assignee/Corporate Source
          Inst. Org. Chem., Univ. Muenchen, Munich, Ger
Source
          Chemische Berichte (1971), 104(8), 2412-19 CODEN: CHBEAM; ISSN: 0009-2940
Document Type
          Journal
Language
          German
Abstract
          The cis-7.8-dihalocycloocta-1.3.5-trienes, formed by chlorination or bromination of cyclooctatetraene (I) at -60° in CH2Cl2, were
          dehydrohalogenated in situ by KOBu-tert at -45° to give 85% bromocycloocatetraene (II) and 74-83% chlorocycloocatetraene, resp.
          Reaction of cyclooctatetraenyllithium with iodine gave iodocyclooctatetranene. Methoxy-, phenoxy-, methyl-, and
          phenylcyclooctatetraene were also prepared from I or II by known methods.
L5 ANSWER 53 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
Title
          Further contributions to the mechanism of the halocyclooctatetraene rearrangement
Author/Inventor
          Konz, Will E.; Hechtl, Wolfgang; Huisgen, Rolf
Patent Assignee/Corporate Source
          Inst. Org. Chem., Univ. Muenchen, Munich, Fed. Rep. Ger.
Source
          Journal of the American Chemical Society (1970 ), 92(13), 4104-5 CODEN: JACSAT: ISSN: 0002-7863
Document Type
          Journal
Language
```

The position of the Br in trans-β-bromostyrene, which was formed from bromocyclooctatetraene (I), was studied. I was brominated

English Abstract to obtain (via II) 1.4-dibromocyclooctatetraene (III), which was converted to the dimethyl derivative by Me2LiCu. III was gas chromatographed to obtain trans-p,β-dibromostyrene. There was a 1,3-migration of the Br atom.

L5 ANSWER 54 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN Title Kinetics and mechanism of the rearrangement of bromocyclooctatetraene to trans-β-bromostyrene Author/Inventor Huisgen, Rolf; Konz, Will E. Patent Assignee/Corporate Source Inst. Org. Chem., Univ. Muenchen, Munich, Fed. Rep. Ger. Journal of the American Chemical Society (1970), 92(13), 4102-4 CODEN: JACSAT: ISSN: 0002-7863 Document Type Journal Language English

A rearrangement mechanism was proposed and discussed in which the valence tautomerization of bromocyclooctatetraene (I) to 1bromobicyclo[4.2.0]octa- 2,4,6-triene (II) was followed by ionization to the homocyclopropenium salt. Ion recombination produced the cyclobutene derivative III, which formed trans-8-bromostyrene by a conrotatory ring opening. Exchange expts, with AgOAc, LiCIO4. MeOH, and Lil indicated a reversible ionization in the rate-determining step, which was verified by the effect of the solvent on the rate. However, another step (I → II) became rate-determining at high solvent polarity. First-order kinetics were observed and rate consts, were calculated for the reaction.

1.5 ANSWER 55 OF 60 CAPILIS COPYRIGHT 2008 ACS on STN

Evidence for different valence tautomers of bromocyclooctatetraene

Author/Inventor

Abstract

Huisgen, Rolf; Konz, Will E.; Gream, George E. Patent Assignee/Corporate Source

Inst. Org. Chem., Univ. Muenchen, Munich, Fed. Rep. Ger. Source

Journal of the American Chemical Society (1970), 92(13), 4105-6 CODEN: JACSAT; ISSN: 0002-7863 Document Type

Journal Language

English

Abstract 1- and 7- Substituted bicyclic tautomers were intermediates in the reactions of bromo- (I) and chlorocyclooctatetrane (II) with 4phenyl-1,2,4-triazoline-3,5-dione (III). A solution of II and III gave 27% IV (R = H, R' = CI) and 30% IV (R = CI, R' = H). I was heated with III to form 12% IV (R = H, R' = Br), 25% IV (R = Br, R' = H), trans-β-bromostyrene, and V. I competed with 1- and 7bromobicyclo[4.2.0]octatriene for the strong dienophile III.

L5 ANSWER 56 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

Title Intermediate occurrence of 1,2- dehydrocyclooctatetraene

Author/Inventor Krebs, A.

Patent Assignee/Corporate Source

Univ. Heidelberg, Germany Source

Angew. Chem. (1965), 77(21), 966

Document Type Journal

Language Abstract

> Bromocyclooctatetraene (I) treated with a suspension of Me3COK in Et2O at room temperature 70 hrs. gave a brown powder, insoluble in Et2O and C6H6. The powder was distilled in vacuo to give 16% tert-butoxycyclooctatetraene (II), b0.05 37-8°. The residue was chromatographed on SiO2 with CCl4 to give 9% naphtho[2,3]cyclooctatetraene (III), m. 113-14°. Hydrolysis of II gave cycloocta-1,3,5-trien-7-one, and hydrogenation gave tert-butoxycyclooctane. Oxidation of III gave benzene-1,2,4,5- tetracarboxylic acid. Dehydrobromination of I by treating with tetraphenylcyclopentadienone or PhN3 gave 72% 1.2.3.4 tetraphenylbenzo[5,6]cyclooctatetraene, m. 241-2°, or 38% 1-phenyl-1,2,3-triazolo[4,5]cyclooctatetraene, m. 67.5-8°, resp., which indicates the occurrence of the cyclooctyne compound as an intermediate.

15 ANSWER 57 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

Title Cyclooctatriene

Author/Inventor

Sanne, Walter: Schlichting, Otto

```
        Patent Assignee/Corporate Source
        Badsche Anilin - & Soda-Fabrik Akt -Ges.

        Document Type
Patent
        Patent

        Language
Unavailable
        Unavailable

        Patent Information
        PATENT NO.
        DATE

        PATENT NO.
        DATE
        APPLICATION NO.
        DATE

        DE 1034626 bit 19580724
        DE 1996-6942186
        19561019
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Patent Number (1)
DE 1034626
Patent Publication Date (1)
19580724
Application Number (1)
DE 1956-B42186
Application Date (1)

19561019 Abstract

1.3,6-Cyclooctatriene (I) was obtained in good yield by reducing cyclooctateraene (II) in aqueous solution with a slight excess of activated Zn in the presence of 0.6 to 0.2 equits, of alkaline bases. A solution of Cyclo 4.2 in water 10 was added af 55° to a stirred mixture of II 624, alc. 950, water 200, and 91% Zn dust 450 parts. NaOH (40%) 50 parts was added slowly to the mixture while the temperature rose to 75°-50." The mixture was neutralized with 25% HZSO4 and steam distilled After cliution of the distillate 2000 with water 6000-8000, the upper layer, containing runde 1617 was separated, dried and distilled to 50th pure 1528 parts, b58 64-5°, n240 1.5056. Alternatively, the alkaline mixture was cooled, diluted with water 8000 parts and the separated corded distilled to obtain pure II ns 8.4% yield.

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L5 ANSWER 58 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
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Title

Monohalo derivatives of cyclooctatetraene
Author/Inventor
Reichender, Franz; Dury, Karl
Patent Assignee/Corporate Source

Badische Anilin- & Soda-Fabrik Akt.-Ges Document Type Patent

Language Unavailable

Unavailable

PATENT NO.	DATE	APPLICATION NO.	DATE
DE 1035648	19580807	DE 1957-B43588	19570220

Patent Number (1)
DE 1035648
Patent Publication Date (1)
19580807
Application Number (1)
DE 1957-B43588
Application Date (1)
19570220

Abstract

The title compds, are prepared by reaction of a 7.8-dihab bicyclo(0.2.4/bycloocha-2.4-diene (i) in the presence of an inert organic solvent, e.g. petr. ether, cyclobhaxane, cyclooctane, C6H6, toluene, Me2NOCH, N-methyl-z-pyrrolidone, doxane, tetrahydrotrura (III), and their mixts, with an alkall metal derivative of acetylene hydrocarbons, e.g. Na acetylde (III), Li acetylde, K (ivnjacetylde and others, at -20 to 60°. To 90 g. I (halogen = CI) in 100 g. II is added at 0-10° with stirring 50 g. III in 500 g. II, the mixture stirred 3 hrs. at room temperature and another 1-2 hrs. at 60°, cooled, mixed with ice H2O, extracted with E120°, dided, the E120° apparated, and the residue distilled to give 35% monochlorocycloctatetraene, b5 50-2°, and 6.5 g. dis-β-chlorostyrene. Analogously is overared the mono-Br derivative b. 15 39-45°.

L5 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN Title

Cyclooctatetraene derivatives
Author/Inventor
Cope, Arthur C.; Burg, Marion
Patent Assignee/Corporate Source
Merck & Co., Inc.
Document Type
Patent
Language

Unavailable Patent Information

PATENT NO.	DATE	APPLICATION NO.	DATE
US 2784240	19570305	US 1952-328255	19521227

Patent Number (1)
US 2784240
Patent Publication Date (1)
19570305
Application Number (1)
US 1952-328255
Application Date (1)
19521227

Abstract

Mono-Cl and mono-Br derivs, of cyclocotatetraene are prepared by dehydrohalogenation between the cyclocotatetraene dihalde (J) and a base at low temperature (Idchholde) (J nucle) in 100 ml dy either was treated under N with 0.11 mole PIAL with vigorous stirring and cooling over 45 min. at .5 to .2° the mixture stirred 10 hm, 100 ml. cold H2O added, the orange layer washed with H2O and the H2O washing extracted with H2O and the H2O washing extracted with H3O ml. and the extract dried and distilled gave 3.6 dg, monochlorocyclocotatetraene, b5.5 50-1°, d25 1.199°, nl.25 1.5342, MD 39.70. Bromocyclocotatetraene (6.6 g.), b1.8 92.5-3°, nD25 1.5870, d25 1.4206, MD 43.26, was also obtained in like mainrer. Monochlorocyclocotatetraene (1.3° g.) and a tew mg. hydroquinone refluxed under N at 200° 2 hm, alve 1.25 g. de-Pi-chrotosytene (1.50 S.5.5°) and nD25 1.5762. Cis-Pi-chrostytene (150 mg.) and 3 mg. PCIS heated at 20-305° 2 hms. in a sealed tube gave cis- and trans-Pi-chlorostytene, nD25 1.5762. Cis-Pi-chrostytene (150 mg.) and 3 mg. PCIS heated at 20-305° 2 hms. in a sealed tube gave cis- and trans-Pi-chlorostytene, nD25 1.5762. Disp-chlorostytene, nD25 1.6052, was obtained similarly, β-todostytene was prepared from 1.38 g. chlorocyclocotatetraene. 195 g. Nal, and a tev mg. hydroquinone in 11 ml. acchoro erfluxed under N 24 hms. giving 72% β-lodostytene, b174°, nD25 1.6395. Li diethylamide and Li 2,6-dimethylpiperidine may be used instead of phenylifithium.

L5 ANSWER 60 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN Title

Cylic polyolefins, XIX. Chloro- and bromocyclooctatetraenes

Author/Inventor Cope, Arthur C.; Brug, Marion

Patent Assignee/Corporate Source

Massachusetts Inst. of Technol.. Cambridge

Source
Journal of the American Chemical Society (1952), 74, 168-72 CODEN: JACSAT; ISSN: 0002-7863

Document Type

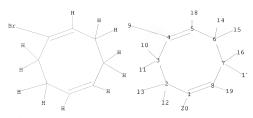
Journal Language

Unavailable

Abstract

cf. C.A. 46, 5600i, 9528d. Evidence supporting the bridged-ring structure for cyclooctatetraene dichloride (I) and dibromide (II) was obtained by oxidation of I to 3,4-dichloro-cis-1,2-cyclobutanedicarboxylic acid (IV). Dehydrohalogenation of I and II with PhLi reopened the bridged ring to give chlorocyclooctatetraene (V) and the Br compound (VI); yields 26 and 33%, resp. Hydrogenation of V and VI over Pt oxide yielded cyclooctane (VII), m. 8-11° and 8.0-11.7°, resp., nD25 1.4560 and 1.4555. (M.ps. are corrected, b.ps. uncor.). Dry Cl (64.5 g.) in 200 cc. CCl4 (prepared at -20 °) added dropwise during 1.5 hrs. to 200 cc. CCl4 at -35 to -25° containing 86 g. cyclooctatetraene (VIII), the mixture stirred 1 hr., let come to room temperature under N, and evaporated in vacuo vielded 111 g. J. b2.7 73-4°, nD25 1.5382, d425 1.2514, f.p. 2.3°, I forms a solid dimer on standing at room temperature I (10 g.) in 100 cc. Me2CO added during 45 min. to 83 g. KMnO4 in 1 l. Me2CO and 400 cc. water at 3-5°, the mixture stirred 8 hrs., let stand 33 hrs. at room temperature, filtered, and the filtrate concentrated to 0.5 volume in vacuo without heating and extracted with Et2O. yielded 4.3 g, IV, m. 176.8-8° (decomposition). I on ozonization yielded 35% IV. IV (426 mg.) in 4 cc. water containing 0.80 g. NaOH hydrogenated 24 hrs. at room temperature and pressure over 0.5 g. Raney Ni W-7 yielded 7.7% cis-1,2cyclobutanedicarboxylic acid (IX), m. 139°. Br (81 g.) in 100 cc. CH2Cl2 added during 1.5 hrs. to 52 g. VII in 150 cc. CH2Cl2 at -15 to -8° yielded 111 g. II, m. 34.0-4.8°. PhLi (0.111 mole) in 270 cc. Et2O added during 45 min, to 17.5 g. I in 100 cc. Et2O at -5 to -2°, the mixture stirred 3 hrs. (ice-salt bath) and 7 hrs. while warming to room temperature, 100 cc. cold water added, and the solution extracted with Et2O yielded 3.66 g, V, b5.5 51-2°, nD25 1.5542, d425 1.1199, MRD 39.70 (calculated 39.94). II (21 g,) in 100 cc. Et2O and 0.078 mole PhLi in 270 cc. Et2O yielded 4.64 g. VI, b1.8 52.5-53°, nD25 1.5870, d425 1.4206, MRD 43.26 (calculated 42.84). V (1.37 g.) and a few mg. p-C6H4(OH)2 (X) refluxed 2 hrs. under N (bath temperature 200-10°) yielded 1.25 g. cis-β-chlorostyrene (XI), b3.5 59°, nD25 1.5762, d425 1.1046; which on hydrogenation yielded PhEt, nD25 1.4923; oxidation of XI with CrO3 yielded BzOH. XI (150 mg.) and 3 mg. PCI5 heated in N 2 hrs. at 200-35° (sealed) yielded a mixture of XI and the trans compound VI (0.75 g.) and X heated 0.5 hrs. under N yielded 0.63 g. β-bromostyrene, b0.65 55-6°, nD25 1.6055, fragrant odor. V (1.38 g.), 1.95 g. Nal, and X in 11 cc. Me2CO refluxed 24 hrs. under N yielded 1.65 g. β-iodostyrene, b1 74°, nD25 1.6585. Ultraviolet absorption spectra are given.

.



chain nodes :

9 10 11 12 13 14 15 16 17 18 19 20

ring nodes :

1 2 3 4 5 6 7 8

chain bonds :

1-20 2-12 2-13 3-10 3-11 4-9 5-18 6-14 6-15 7-16 7-17 8-19

ring bonds :

1-2 1-8 2-3 3-4 4-5 5-6 6-7 7-8

exact/norm bonds :

1-2 1-8 2-3 3-4 4-5 5-6 6-7 7-8

exact bonds :

1-20 2-12 2-13 3-10 3-11 4-9 5-18 6-14 6-15 7-16 7-17 8-19

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 15:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS

1 ANSWERS

L6 STRUCTURE UPLOADED

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L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

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L9 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

Title Preparation of 1,5-cyclooctadiyne and 1,3,5,7-cyclooctatetraene from 1,5-cyclooctadiene Author/Inventor

Detert, Heiner; Rose, Bernd; Mayer, Winfried; Meier, Herbert

Patent Assignee/Corporate Source

Inst. Org. Chem., Univ. Mainz, Mainz, D-55099, Germany

Chemische Berichte (1994), 127(8), 1529-32 CODEN: CHBEAM: ISSN: 0009-2940 Document Type

Journal

Language German

Abstract

Bromination of 1.5-cyclooctadiene and stepwise dehydrobromination with KOCMe3 and then KOCMe3/18-crown-6 yields 1.5cyclooctadivne (5). Prolonged interaction with the base causes complete transformation to cyclooctatetraene. Divne 5 and even more the intermediate 1-bromo-1-cyclooctenyne are highly reactive dienophiles. The cycloadducts formed with 1,3-cyclohexadiene, carbon disulfide, and tetraphenylcyclopentadienone were isolated and characterized. Treatment of 5 with titanium tetrachloride induces a vigorous polymerization

19 ANSWER 2 OF 6 CAPILIS COPYRIGHT 2008 ACS on STN Title

Trimethylsilylcyclooctadiene-transition metal complexes: metal-catalyzed protodesilylation of cyclic vinylsilanes, and transfer hydrogenation promoted by the displaced silvl group

Author/Inventor

Bandodakar, Balachandra S.; Nagendrappa, Gopalpur

Patent Assignee/Corporate Source

Dep. Chem., Bangalore Univ., Bangalore, 560 001, India Source

Journal of Organometallic Chemistry (1992), 430(3), 373-83 CODEN; JORCAI; ISSN: 0022-328X

Document Type

Journal Language

English

Abstract

Complexes of 1-trimethylsilyl-1,5-cyclooctadiene (TMS-COD) with Aql, Rhl, PdII and PtII have been prepared and characterized. The distortion in their structures in comparison with the near sym, structures of the corresponding, 1,5-cyclooctadiene (COD) complexes, which is obviously attributable to the presence of vinylic SiMe3 group, is clearly indicated by their 1H and 13C NMR spectral characteristics. The silver complex is somewhat unstable, but the other complexes are quite stable. An unstable Cul complex that could not be satisfactorily characterized was also obtained. If appropriate conditions for the preparation of Rh and Pd complexes are not maintained, desilylation occurs, accompanied by reduction of COD to cyclooctene by transfer of hydrogen from the solvent alc. The displaced silicon-containing moiety seems to enhance the transfer hydrogenation. Attempts to prepare a Rull complex resulted in the formation of a complex of desilylated diene (Rull-COD).

L9 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

Title

A simple preparation of cyclic vinylic bromides (1-bromocycloalkenes and 1-bromo-1,5-cyclooctadiene) from 1,2dibromocycloalkanes

Author/Inventor

Bandodakar, Balachandra S.; Nagendrappa, Gopalpur

Patent Assignee/Corporate Source

Dep. Chem., Bangalore Univ., Bangalore, 560 001, India Source

Synthesis (1990), (9), 843-4 CODEN; SYNTBF; ISSN: 0039-7881 Document Type

Journal

Language

English

Abstract 1,2-Dibromocyclopentane, -cyclohexane, -cycloheptane, -cyclooctane, and -cyclododecane, and 5,6-dibromocyclooctene are smoothly dehydrobrominated to the corresponding 1-bromocycloalkenes in 45-84% yield using morpholine-DMSO in C6H6 or EtOH.

L9 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

9-Oxabicyclo[6.1.0]nonynes

Author/Inventor

Title

Mayer, Winfried; Meier, Herbert

Patent Assignee/Corporate Source

Inst. Org. Chem., Univ. Mainz, Mainz, D-6500, Fed. Rep. Ger.

Source

Chemische Berichte (1989). 122(3), 509-17 CODEN: CHBEAM: ISSN: 0009-2940

Document Type

Journal

Language

Abstract

Semiempirical quantum mechanics (MNDO) and force field calcns. (MM2) reveal that two diastereometic conformations of low energy exist for each of the three isomeric cis-9-oxabicyclo[6.1.0]nonynes I (n, m = 0.4; 1,3; 2,2). I are accessible by the selenadiazole method or by dehydrobromination. Conformational anal, by NMR spectroscopy confirms the predicted equilibrium for I (n = 1, m = 3); for I (n = 0 m = 4) both conformers even at -60 °C show a fast equilibration by inversion of the eight-membered ring. and only one conformation is populated.

19 ANSWER 5 OF 6 CAPILIS COPYRIGHT 2008 ACS on STN

Title Photolysis of some 1-substituted cycloocta-1.5-dienes; synthesis of 1-fluorotricyclof3.3.0.02.6loctane

Author/Inventor

Cotsaris, Evangelo; Della, Ernest W. Patent Assignee/Corporate Source

Sch. Phys. Sci., Flinders Univ. South Australia, Bedford Park, 5042, Australia

Source

Australian Journal of Chemistry (1980), 33(11), 2561-4 CODEN: AJCHAS: ISSN: 0004-9425

Document Type Journal

Language English

Abstract

In a study of the photolysis of several of cycloocta-1,5-diene derivs, as possible precursors of bridgehead-substituted tricyclo[3,3,0,02,6]octanes, only 1-fluoro-1,5-cyclooctadiene successfully underwent photocyclization, giving 1fluorotricyclo[3,3,0,02,6]octane, 1-Bromo-1,5-cyclooctadiene suffered fission of the carbon-bromine bond, while 1,5-cyclooctadiene-1- carbonitrile afforded a mixture of at least 4 unsated isomers

L9 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

Title

Importance of the aromatic ring in adrenergic amines. 2. Synthesis and adrenergic activity of some nonaromatic six- and eightmembered ring analogs of β-phenylethanolamine

Author/Inventor

Grunewald, Gary L.; Grindel, Joseph M.; Patil, Popat N.; Salman, Kadhim N.

Patent Assignee/Corporate Source

Sch. Pharm., Univ. Kansas, Lawrence, KS, USA Source

Journal of Medicinal Chemistry (1976), 19(1), 10-16 CODEN; JMCMAR; ISSN: 0022-2623 Document Type

Journal

Language

English

Abstract

Title analogs 2-cyclohexyl-2-hydroxyethylamine-HCl (I) [57559-32-7] and 2-cyclooctyl-2-hydroxyethylamine-HCl (II) [57559-31-6] and unsatd, analogs 2-(cyclohexen-4-yl)- [57559-51-0], 2-cyclooctatetraenyl- [57559-48-5], 2-cyclooctenyl- [57559-49-6], 2cycloocta-1,3-dien-2-yl-[57559-50-9], and 2-(cycloocta-1,5-dien-2-yl)-2-hydroxyethylamine-HCI [57230-10-1] were prepared by conversion of the corresponding aldehydes to the cyanohydrins, followed by reduction. All compds, had indirect adrenergic activity on the rat vas deferens and on the reserpinized rat vas deferens they potentiated the effects of exogenous norepinephrine. The more saturated the ring moiety, the greater the affinity of the compound was for the amine uptake site of the vas deferens. There was no evidence of interaction of the drug and the uptake site involving π-complex formation.